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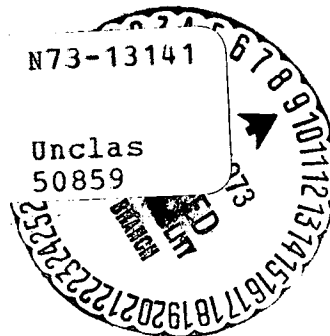
Translation of: "Etude des évolutions chimiques
dans une couche de mélange hydrogene - air,"
Office National d'Etudes et de Recherches
Aérospatiales, T.P. No. 981, 1971, pp. 1-4.

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CHEMICAL TRANSFORMATIONS IN A HYDROGEN-AIR MIXING LAYER

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ABSTRACT. Studies the chemical evolution in an air - hydrogen mixing layer. The confluence of two parallel flows of air and hydrogen is examined numerically in order to determine the conditions of self-ignition in the mixing layer. The calculations show that the reaction zone is limited to the stoichiometric region. For the two streams at the same temperature, the ignition length can be evaluated by neglecting the effects of lateral diffusion.

1. INTRODUCTION

The turbulent mixing layer which develops between two parallel flows downstream of their confluence can be the site of chemical transformations if the two gases react with each other. In this case, determination of the conditions for auto-ignition within the mixture is a problem of general practical interest.

The present study examines the idealized case of the confluence of uniform flows of air and hydrogen, assumed to have no initial boundary layers (Fig. 1). The numerical solution of the problem is handled within the framework of the usual description of turbulent flows by mean values, and also by introducing into the corresponding computer program the mechanism of chemical reaction between hydrogen and air.

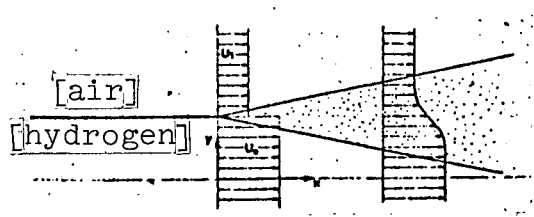


Fig. 1. Mixing configuration examined.

2. BASIC EQUATIONS AND HYPOTHESES

The conservation equations for the $(N+3)$ fundamental quantities (mass, momentum, total enthalpy, partial masses of the N species present) can be written for a turbulent, isobaric, mean steady-state flow as:

$$\frac{\partial}{\partial x} \bar{\rho u} + \frac{1}{Y_j} \frac{\partial}{\partial y} (Y_j \bar{\rho v}) = 0 \quad (1)$$

$$\frac{\partial}{\partial x} \bar{\rho u^2} + \frac{1}{Y_j} \frac{\partial}{\partial y} (Y_j \bar{\rho v u}) = 0 \quad (2)$$

$$\frac{\partial}{\partial x} \bar{\rho u H} + \frac{1}{Y_j} \frac{\partial}{\partial y} (Y_j \bar{\rho v H}) = 0 \quad (3)$$

$$\frac{\partial}{\partial x} \bar{\rho u C_i} + \frac{1}{Y_j} \frac{\partial}{\partial y} (Y_j \bar{\rho v C_i}) = \dot{w}_i \quad (4)$$

$(i = 1, \dots, N)$

Where the molecular-transport terms are neglected.

Assuming the fluctuations in the quantities u, v, H, C_i are small with respect to the corresponding mean values (as well as $y, \bar{v}$, and the derivatives with respect to X), Equations (2) to (4) can be written as:

$$\bar{\rho u} \frac{\partial \bar{Q}}{\partial x} + \bar{\rho v} \frac{\partial \bar{Q}}{\partial y} = S_Q - \frac{1}{Y_j} \frac{\partial}{\partial y} [Y_j \bar{\rho} \overline{v' Q'}] \quad (5)$$

where $\bar{Q}$ represents the mean value of $[u, H]$, and the C_1, S_q the corresponding source terms ($S_q = 0$ for u and H). Because of the decomposition into mean and fluctuational components, turbulent exchange fluxes $\overline{q'v'}$ appear in the right-hand member of Equation (5). Elimination of the fluctuational quantities is accomplished by means of a generalization of Boussinesq's formula:

$$\overline{Q'v'} = -\epsilon_q \frac{\partial \bar{Q}}{\partial y} \quad (6)$$

($Q = U, H, C_1, \dots, C_n$),

where the exchange coefficients $[\epsilon_q]$ depend on the local properties of the flow. Expressions for $[\epsilon_u]$ ("turbulent kinematic viscosity") based on Prandtl's mixing-length hypothesis are the only ones used in the present study. Thus:

$$\epsilon_u = l^2 \left| \frac{\partial \bar{u}}{\partial y} \right| \quad (7)$$

or

$$\epsilon_u = kb |u_1 - u_0| \quad (8)$$

where the mixing length l is assumed to be proportional to the thickness b of the mixing layer. The coefficients $[\epsilon_h]$ of the static enthalpy h , and $[\epsilon_c]$ of the concentrations $C_1, \dots, C_n$ are defined from $[\epsilon_u]$ by means of the turbulent Prandtl and Schmidt numbers.

$$\epsilon_h = \frac{\epsilon_u}{Pr_t}, \quad \epsilon_c = \frac{\epsilon_u}{Sc_t} \quad (9)$$

The total enthalpy-exchange flux is expressed by the coefficients $[\epsilon_h]$ and $[\epsilon_u]$ by:

$$\overline{H'v'} = \overline{(h' + \bar{u}u')v'} = -\epsilon_h \frac{\partial \bar{h}}{\partial y} - \bar{u} \epsilon_u \frac{\partial \bar{u}}{\partial y} \quad (10)$$

In addition, there is practical interest in replacing the total enthalpy H in the energy equation by the static temperature, using:

$$dH = c_p dT + \sum_i h_i dC_i + u du \quad (11)$$

Thus, (N+2) equations are obtained in terms of the mean values:

$$\bar{\rho} \frac{\partial \bar{u}}{\partial x} + \bar{\rho} \frac{\partial \bar{u}}{\partial y} = \frac{1}{\gamma} \frac{\partial}{\partial y} \left[\gamma^j \bar{\rho} \varepsilon_u \frac{\partial \bar{u}}{\partial y} \right] \quad (12)$$

$$\bar{c}_p \left\{ \bar{\rho} \frac{\partial \bar{T}}{\partial x} + \bar{\rho} \frac{\partial \bar{T}}{\partial y} \right\} = \frac{1}{\gamma} \frac{\partial}{\partial y} \left[\gamma^j \bar{\rho} \varepsilon_h \bar{c}_p \frac{\partial \bar{T}}{\partial y} \right] + \bar{\rho} \varepsilon_u \left(\frac{\partial \bar{u}}{\partial y} \right)^2 + \bar{\rho} \varepsilon_h \frac{\partial \bar{T}}{\partial y} \sum_i \bar{c}_{p_i} \frac{\partial \bar{x}_i}{\partial y} - \sum_i \bar{h}_i \bar{w}_i \quad (13)$$

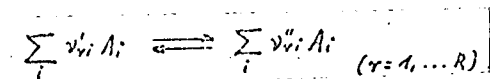
$$\bar{\rho} \frac{\partial \bar{c}_i}{\partial x} + \bar{\rho} \frac{\partial \bar{c}_i}{\partial y} = \frac{1}{\gamma} \frac{\partial}{\partial y} \left[\gamma^j \bar{\rho} \varepsilon_c \frac{\partial \bar{c}_i}{\partial y} \right] + \bar{w}_i \quad (14)$$

$$(i = 1, \dots, N)$$

The chemical-production terms $\bar{w}_i$ appearing in the right-hand members of Equations (13) and (14) are expressed as functions of T and the $c_1, \dots, c_N$ by the fundamental relation of chemical kinetics:

$$\bar{w}_i = \sum_r (\gamma''_{ri} - \gamma'_{ri}) A_r \left[\bar{h}'_r T \prod_j \left(\frac{\bar{c}_j}{A_j} \right)^{\gamma'_{rj}} - \bar{h}''_r T \prod_j \left(\frac{\bar{c}_j}{A_j} \right)^{\gamma''_{rj}} \right] \quad (15)$$

where γ'_{ri} and γ''_{ri} are the stoichiometric coefficients of species A_i in the T reaction:



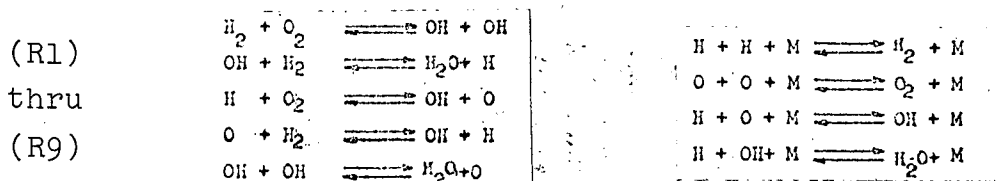
The speed $\bar{h}'_r$ of the forward reaction is assumed to be of the form:

$$\bar{h}'_r = B_r T^{u_r} e^{-\frac{E_r}{RT}} \quad (16)$$

while the speed $\bar{h}''_r$ of the inverse reaction is determined from $\bar{h}'_r$ and the equilibrium constant $K_{p_r} = \exp \left\{ -\frac{\Delta(h^\circ - T \Delta s^\circ)}{RT} \right\}$ for the T reaction:

$$\bar{h}''_r = \bar{h}'_r \left(\frac{P}{P^\circ} \right)^{\alpha_r} e^{\frac{\Delta(h^\circ - T \Delta s^\circ)}{RT}} \quad \alpha_r = \sum_i (\gamma''_{ri} - \gamma'_{ri}) \quad (17)$$

Of all the reactions determining the ignition process for a hydrogen-air mixture, the following are considered in the present calculations:



Furthermore, the high-temperature reactions among the constituents of air are taken into account when the numerical calculation is extended to equilibrium. The numerical values used are those given in [1] for the $H_2 - O_2$ system, and in [2] for the remaining reactions.

3. METHOD OF SOLUTION

The solution method is based on numerical integration of the (N+2) equations (12) through (14). To facilitate the calculation, a change of variables is made by introducing a stream function ψ which satisfies Equation (1):

$$\psi^j \frac{\partial \psi}{\partial y} = \bar{c} u^j, \quad \psi^j \frac{\partial \psi}{\partial x} = -\bar{c} v^j \quad (18)$$

The transverse velocity V is thus eliminated.

The K mass balances (K is the number of chemical elements present) allow the number of the diffusion equations (14) to be reduced from N to $(N - K + 1)$. The total number of equations to be integrated is thus reduced to $(N - K + 3)$. In the present case, where $N = 9$ (species $H, N, O, OH, NO, H_2O, H_2, N_2, O_2$) and $K = 3$ (elements H, N, O), there are still seven^{*)} equations to be solved simultaneously.

The numerical solution is carried out in the transformed $[x - \psi]$ plane, using an explicit finite-difference program [3]; integration is performed in the X direction along the stream lines, noting at each step the boundary conditions imposed at the edge of the mixing layer. The integration step Δx is determined from the most severe of the criteria for stability and for maximum increase in the temperature or concentrations over that step.

^{*)} There are nine: 7 in (14), plus (12) and (13).

4. RESULTS OF THE CALCULATION

When the mixing layer develops without chemical reaction ($\dot{w}_i = 0$), the system of equations (12) to (14) is considerably simplified -- the total number of equations to be integrated can be reduced to 3.

Figure 2 shows similitude profiles for H_2 concentration, calculated with expressions (7) and (8) for ξ/δ . Their behavior is quite close to the corresponding incompressible-flow solutions of Tollmien and of Goertler, respectively.

Ignition of a mixture of air and hydrogen is characterized by the phenomenon of isothermal induction before the appearance of the exothermic phase of the reaction. The isothermal induction period is caused by rapid changes in the chemical species H, O, OH, and H_2O , due principally to Reactions (R1) to (R5), while the rapid temperature rise at the end of induction is to be attributed to the recombination reactions (R6) to (R9).

Variations in the times for induction and combustion as functions of the initial composition (represented by the richness ϕ) of a mixture at 1000°K is shown in Figure 3, where the two time periods are characterized by relative increases in temperature of 10% and 90% respectively; the induction period can also be located by the maximum in the H concentration. As a result of the relatively slow variation of this period (which varies here approximately as $e^{C_0/\phi}$), it is to be expected that within the mixing layer, where ϕ varies between 0 and CO_{st} , the ignition phenomena occur in the stoichiometric region, at least in the isothermal case.

If, on the other hand, the temperatures of the two flows are different, one may expect more marked lateral diffusion than in the preceding case because of the strong dependence of chemical production on temperature. An illustration is given in Figure 4 for $\phi = 1$; the strong variation in the ignition period is connected to that of the inverse of the Arrhenius term of Equation (R3):

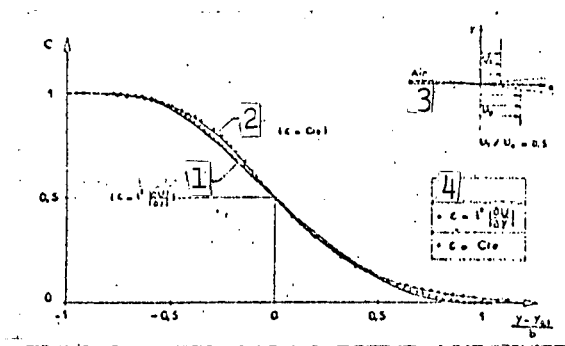


Fig. 2. Similitude profiles for hydrogen cone concentration.

1 - Tollmien's theory; 2 - Goertler's theory; 3 - Hydrogen; 4 - Finite-difference calculation.

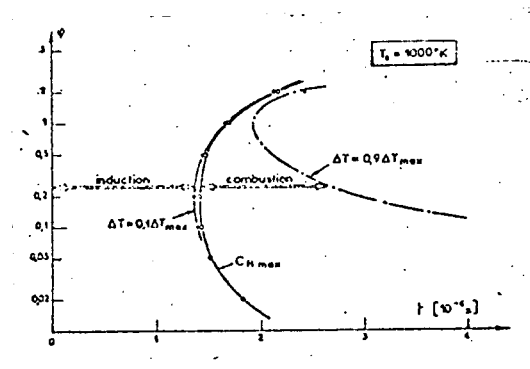


Fig. 3. Ignition time as function of ϕ .

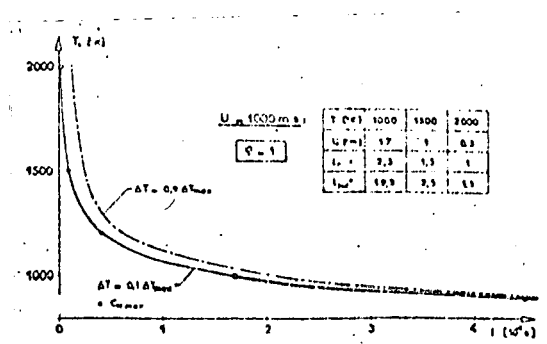


Fig. 4. Chemical times as functions of initial temperature, (Reaction H_2 - Air, $\phi = 1$).

$$t_i \sim T e^{\frac{6010}{T}}$$

The distinctly more moderate variation of the period of exothermic reaction (represented by the horizontal displacement between the two curves) is attributed to very weak temperature-dependence of the velocities of the recombination reactions.

In Figure 5, the isotherms and the curves in the physical plane showing constant concentrations of atomic hydrogen have been obtained for mixture of two flows initially at the same temperature, 1000°K. As in the preceding diffusionless case, these curves show a quasi-isothermal region with strong growth in H, O, OH and H₂O, followed by the zone of exothermic reactions. The maximum concentration increase lies around the stoichiometric line, $\varphi = 1$ so that behavior close to that occurring in the absence of lateral diffusion should be expected along this line. As Figure 6 shows for the behavior of temperature T and concentration C_H, this agreement extends into the region of active combustion. Thus, for an initially isothermal mixing layer, conditions for auto-ignition can be predicted validly by use of a simplified computer program which disregards diffusion of the species created.

5. CONCLUSION

The present example of the numerical calculation of the ignition process has shown that the latter develops mainly in a narrow region around the stoichiometric line. For mixing which is initially isothermal, the ignition and combustion lengths can be evaluated by use of simple relations which involve only the common temperature of the two confluent flows.

In the non-isothermal case, which must still be examined numerically, one must expect an increasing influence of the ratio of the two initial temperatures as it departs from 1.

The influence of initial boundary layers, which could not be

